Computational statistics

Chapter 1: Continuous Optimization

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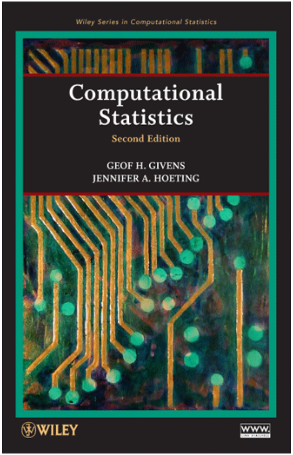
Computational statistics

- Modern methods in statistics and econometrics rely heavily on computational methods, for instance,
  - Nonlinear optimization
  - Monte Carlo simulation
  - Resampling techniques (bootstrap, cross-validation)
  - Nonparametric density estimation and smoothing
  - Machine Learning, data mining, big data analysis, etc.
- Computational statistics is a branch of Statistics at the intersection with Computer Science. It concerns the study of efficient procedures for solving statistical problems with computers.

Contents of this course



- Two parts:
  1. Part I: optimization
  2. Part II: simulation
- We will use the R programming language (free, flexible, large collection of available statistical methods).
- Recommended textbook: G. H. Givens and J. A. Hoeting, *Computational Statistics*, Wiley.

Part I: Optimization

- Many problems in statistics can be seen as optimizing (i.e., minimizing or maximizing) some function, for instance:
  - Maximizing the likelihood
  - Finding the mode of the posterior density, or highest posterior density intervals in Bayesian analysis
  - Minimizing risk in Bayesian decision problems
  - Minimizing empirical risk (error) in machine learning problems, etc.
- For the simplest models (e.g. least-squares linear regression), a closed-form expression of the solution can be found. In most cases, we have to resort to iterative procedures.

Categories of optimization problems

- Continuous vs. combinatorial optimization
- Univariate vs. multivariate
- Unconstrained vs. constrained

Contents of this course (Part I)

1. Optimizing smooth univariate functions: bisection, Newton's method, Fisher scoring, secant method
2. Optimizing smooth multivariate functions: nonlinear Gauss-Seidel iteration, Newton's method, Fisher scoring, Gauss-Newton method, ascent algorithms, discrete Newton method, quasi-Newton methods
3. Combinatorial optimization: local search, ascent algorithms, simulated annealing, genetic algorithms
4. Expectation-Maximization (EM) algorithm for maximizing the likelihood or posterior density

Contents of this course (Part II: simulation)

1. Simulation of probability distributions: probability integral transform, rejection sampling, sampling importance resampling
2. Markov chain Monte Carlo (MCMC) methods: Metropolis-Hastings algorithm, Gibbs sampling, application to Bayesian inference
3. Bootstrap

Overview

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   - Gauss-Newton method
   - Nelder-Mead algorithm

Introduction to optimization

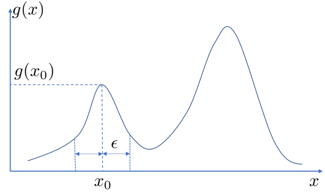
- In this first part, the real-valued function $g : \mathbb{R}^p \rightarrow \mathbb{R}$ to be maximized or minimized will be assumed to be smooth (at least differentiable).
- It may be a likelihood, a profile likelihood, a Bayesian posterior, an error/loss function, or any other function.
- Minimizing g is equivalent to maximizing $-g$.
- Unless otherwise specified, we will consider maximization problems, without loss of generality.

Local vs. global maximum

Definition (Local maximum)

A vector $\mathbf{x}_0$ is a local maximum of g if $\exists\, \epsilon > 0$ such that, for all $\mathbf{x} \in \mathbb{R}^p$,

$$\|\mathbf{x} - \mathbf{x}_0\| \leq \epsilon \Rightarrow g(\mathbf{x}_0) \geq g(\mathbf{x})$$



Definition (Global maximum)

A vector $\mathbf{x}_0$ is a global maximum of g if, for all $\mathbf{x} \in \mathbb{R}^p$,

$$g(\mathbf{x}_0) \geq g(\mathbf{x})$$

Local vs. global maximum (continued)

- We usually want to find a global maximum, but optimization algorithms can only be guaranteed to converge to a local maximum.
- Solution: restart the algorithm from different initial conditions, but we can never be sure to have reached a global maximum.

Fermat's theorem

In general, we will use Fermat's theorem:

Theorem (Fermat's theorem – univariate case)

Let g be a differentiable function from an open interval (a, b) to $\mathbb{R}$. If g has a local maximum at a point $x \in (a, b)$, then $g'(x) = 0$.

or its multivariate generalization:

Theorem (Fermat's theorem – multivariate case)

Let g be a differentiable function from an open set $E \subseteq \mathbb{R}^p$ to $\mathbb{R}$. If g has a local maximum at a point $\mathbf{x} \in E$, then $\mathbf{g}'(\mathbf{x}) = \mathbf{0}$, where

$$\mathbf{g}'(\mathbf{x}) = \left(\frac{\partial g(\mathbf{x})}{\partial x_1}, \ldots, \frac{\partial g(\mathbf{x})}{\partial x_p} \right)^T$$

is the gradient of g at $\mathbf{x}$

Maximum likelihood estimation

- For maximum likelihood estimation, g is the log likelihood function ℓ, and $\mathbf{x}$ is the corresponding parameter vector $\boldsymbol{\theta}$. If $\widehat{\boldsymbol{\theta}}$ is a MLE, it maximizes the log likelihood. Therefore $\widehat{\boldsymbol{\theta}}$ is a solution to the score equation

$$\ell'(\boldsymbol{\theta}) = \mathbf{0},$$

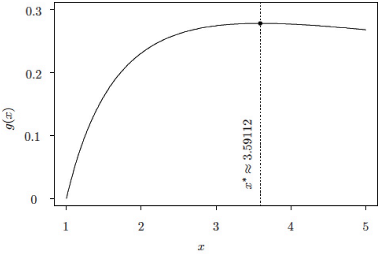
where $\ell'(\boldsymbol{\theta}) = \left(\frac{\partial \ell(\boldsymbol{\theta})}{\partial \theta_1}, \ldots, \frac{\partial \ell(\boldsymbol{\theta})}{\partial \theta_p}\right)^T$ and $\mathbf{0}$ is a column vector of zeros.

- We see that optimization is intimately linked with solving nonlinear equations. Finding a MLE amounts to finding a root of the score equation.
- In general, the maximum of g is a solution to $\boldsymbol{g}'(\mathbf{x}) = \mathbf{0}$.

Univariate Optimization for Smooth g

Example 1

- Maximize
$$g(x) = \frac{\log(x)}{1+x}$$
with respect to x.
- We cannot find the root of $g'(x) = \frac{1+1/x-\log x}{(1+x)^2}$ analytically.



- The maximum of $g(x) = \frac{\log(x)}{1+x}$ occurs at $x^* \approx 3.59112$, indicated by the vertical line.

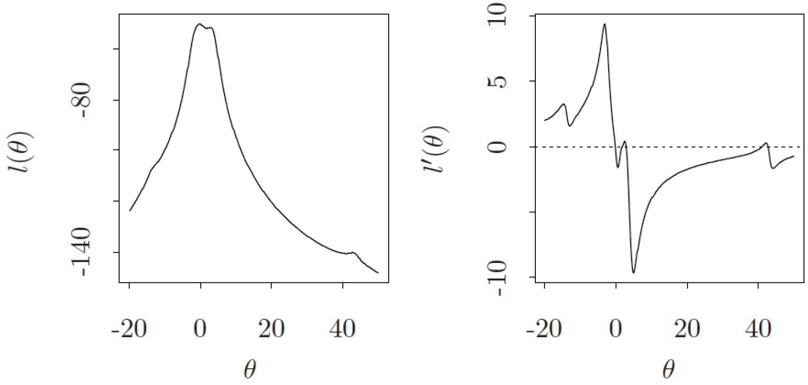
Example 2

- The following data are an i.i.d. sample from a Cauchy$(\theta, 1)$ distribution:
  1.77, -0.23, 2.76, 3.80, 3.47, 56.75, -1.34, 4.24, -2.44, 3.29, 3.71, -2.40, 4.53, -0.07, -1.05, -13.87, -2.53, -1.75, 0.27, 43.21.
- The likelihood function is

$$L(\theta) = \prod_{i=1}^{20} \frac{1}{\pi\left(1 + (x_i - \theta)^2\right)}$$

  Find the MLE for θ.
- The score function $\ell'(\theta)$ has multiple roots requiring numerical solution. (See next slide)

Log likelihood and score function for the Cauchy data



Remark: in this example, the roots of equation $\ell'(\theta) = 0$ correspond to minima and maxima. The maxima satisfy the additional condition $\ell''(\theta) < 0$.

Maximum or minimum? The second derivative test

Univariate case

Suppose $g : \mathbb{R} \mapsto \mathbb{R}$ is twice differentiable and $g'(x) = 0$.

- If $g''(x) > 0$ then g has a local minimum at x.
- If $g''(x) < 0$ then g has a local maximum at x.
- If $g''(x) = 0$ then the test tells us nothing.

Maximum or minimum? The second derivative test

Multivariate case

Suppose $g : \mathbb{R}^p \mapsto \mathbb{R}$ is twice differentiable and $\mathbf{g}'(\mathbf{x}) = 0$. We consider the matrix of second derivatives, called the Hessian matrix:

$$\mathbf{g}''(\mathbf{x}) = \left(\frac{\partial^2 g(\mathbf{x})}{\partial x_i \partial x_j} \right)$$

- If $\mathbf{g}''(\mathbf{x})$ is positive definite (equivalently, has all eigenvalues positive) at $\mathbf{x}$, then g attains a local minimum at $\mathbf{x}$.
- If $\mathbf{g}''(\mathbf{x})$ is negative definite (equivalently, has all eigenvalues negative) at $\mathbf{x}$, then g attains a local maximum at $\mathbf{x}$.
- If $\mathbf{g}''(\mathbf{x})$ has both positive and negative eigenvalues then $\mathbf{x}$ is a saddle point for g.

Iterative methods

- Recall the simple example where we seek to maximize

$$g(x) = \frac{\log(x)}{1+x}$$

  with respect to x.

- We will rely on successive approximations of the solution.
- If we know that the maximum is around 3, it might be reasonable to use $x^{(0)} = 3.0$ as an initial guess, or starting value.
- An update equation will be used to produce an improved guess, $x^{(t+1)}$, from the most recent value $x^{(t)}$, for $t = 0, 1, 2, \ldots$ until iterations are stopped.

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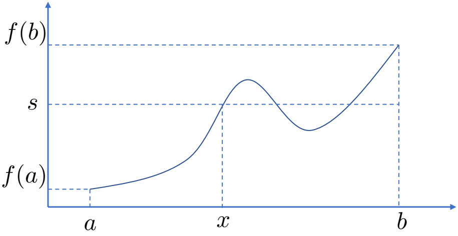
Bisection Method

Intermediate value theorem

- In this section we assume that $g : \mathbb{R} \to \mathbb{R}$ is a univariate function.
- We will use the following theorem:

Theorem (Intermediate value theorem (IVT))

If f is a continuous function whose domain contains the interval $[a, b]$, then for any $s \in [f(a), f(b)]$, there exists $x \in [a, b]$ such that $f(x) = s$.



Bisection Method

- If g' is continuous on $[a_0, b_0]$ and $g'(a_0)g'(b_0) \leq 0$ then by the IVT there exists at least one $x^* \in [a_0, b_0]$ for which $g'(x^*) = 0$; hence, x^* is a local optimum of g.
- To find such a root, the bisection method systematically shrinks the interval from $[a_0, b_0]$ to $[a_1, b_1]$ to $[a_2, b_2]$ and so on, where $[a_0, b_0] \supset [a_1, b_1] \supset [a_2, b_2] \supset \cdots$ are nested intervals.
- If these intervals are chosen to retain $g'(a_i)g'(b_i) \leq 0$, then the ith interval contains a root.

Bisection Method

- Let $a_0 \leq b_0$ such that $g'(a_0)g'(b_0) \leq 0$, and let $x^{(0)} = (a_0 + b_0)/2$ be the starting value.
- The update equations are

$$[a_{t+1}, b_{t+1}] = \begin{cases} [a_t, x^{(t)}] & \text{if } g'(a_t)g'(x^{(t)}) \leq 0 \\ [x^{(t)}, b_t] & \text{if } g'(a_t)g'(x^{(t)}) > 0 \end{cases}$$

and

$$x^{(t+1)} = \frac{a_{t+1} + b_{t+1}}{2}$$

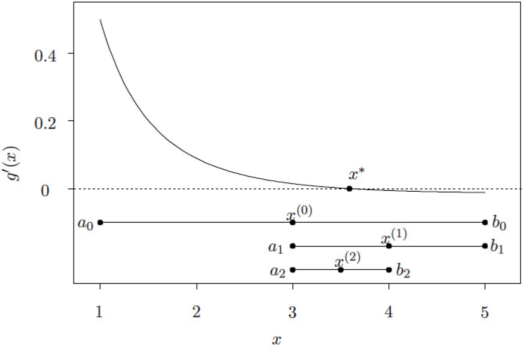
- If g has more than one root in the starting interval, it is easy to see that bisection will find one of them, but will not find the rest.

Example

To find the value of x maximizing

$$g(x) = \frac{\log(x)}{1+x}$$

we might take $a_0 = 1$, $b_0 = 5$, and $x^{(0)} = 3$.



Properties

- For continuous smooth functions, bisection is guaranteed to converge to a root because a root is always in the interval and the length of the interval halves at each iteration.
- However, the method is slow.

Stopping Criteria

- Near the root $g'(x^{(t+1)}) \approx 0$. However, relatively large changes from $x^{(t)}$ to $x^{(t+1)}$ are often seen even when $g'(x^{(t+1)})$ is roughly zero, therefore a stopping rule based directly on $g'(x^{(t+1)})$ is not very reliable.
- On the other hand, a small change from $x^{(t)}$ to $x^{(t+1)}$ is most frequently associated with $g'(x^{(t+1)})$ near zero. Therefore, we typically assess convergence by monitoring $\left|x^{(t+1)} - x^{(t)}\right|$ and use $g'(x^{(t+1)})$ as a backup check.
- The absolute convergence criterion mandates stopping when

$$\left|x^{(t+1)} - x^{(t)}\right| < \epsilon$$

where ϵ is a constant chosen to indicate tolerable imprecision.

Stopping Criteria (continued)

- The relative convergence criterion mandates stopping when iterations have reached a point for which

$$\frac{\left|x^{(t+1)} - x^{(t)}\right|}{\left|x^{(t)}\right|} < \epsilon \tag{1}$$

- This criterion enables the specification of a target precision (e.g., 'within 1%') without worrying about the units of x.
- Preference between the absolute and relative convergence criteria depends on the problem at hand:
  - If the scale of x is huge (or tiny) relative to ϵ, an absolute convergence criterion may stop iterations too reluctantly (or too soon).
  - The relative convergence criterion corrects for the scale of x, but can become unstable if $x^{(t)}$ values (or the true solution) lie too close to zero.
- In this latter case, another option is to monitor relative convergence by stopping when $\frac{\left|x^{(t+1)}-x^{(t)}\right|}{\left|x^{(t)}\right|+\epsilon} < \epsilon$.

Convergence diagnostics

- Also important to include stopping rules that flag a failure to converge:
  - Stop after N iterations, regardless of convergence. Do not devote all affordable iterations to one attempt! Budget time for many smaller attempts, anticipating convergence failures, data corrections, multiple starting values, etc.
  - Could stop if any convergence measure fails to decrease or cycle over several iterations.
  - It is also sensible to stop if the procedure appears to be converging to a point at which $g(x)$ is inferior to another value you have already found (i.e., a known false peak or local maximum).
- Regardless of which such stopping rules you employ, any indication of poor convergence behavior means that $x^{(t+1)}$ must be discarded and the procedure somehow restarted in a manner more likely to yield successful convergence.

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Newton's Method

- Suppose that g' is continuously differentiable and that $g''(x^*) \neq 0$.
- At iteration t, the approach approximates $g'(x^*)$ by the linear Taylor series expansion about $x^{(t)}$:

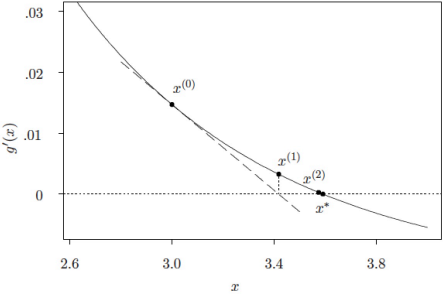
$$0 = g'(x^*) \approx g'(x^{(t)}) + (x^* - x^{(t)})g''(x^{(t)})$$

- Since g' is approximated by its tangent line at $x^{(t)}$, it seems sensible to approximate the root of g' by the root of the tangent line. Thus, solving for the root,

$$x^* \equiv x^{(t+1)} = x^{(t)} - \frac{g'(x^{(t)})}{g''(x^{(t)})} = x^{(t)} + h^{(t)}$$

Example

Function of Example 1: $g(x) = \frac{\log(x)}{1+x}$



Starting from $x^{(0)} = 3.0$, Newton's method quickly finds $x^{(4)} \approx 3.59112$. For comparison, the first five decimal places of x^* are not correctly determined by the bisection method until iteration 19.

Convergence rate

Definition

Let $\epsilon^{(t)} = x^{(t)} - x^*$ be the approximation error at iteration t. A method has convergence of order β if $\lim_{t\to\infty} \epsilon^{(t)} = 0$ and

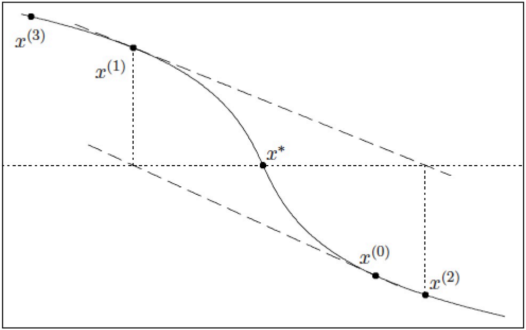
$$\lim_{t\to\infty} \frac{\left|\epsilon^{(t+1)}\right|}{\left|\epsilon^{(t)}\right|^{\beta}} = c$$

for some constants $c \neq 0$ and $\beta > 0$.

- Higher orders of convergence are better in the sense that precise approximation of the true solution is more quickly achieved.
- Newton's method has quadratic convergence order, $\beta = 2$
- Unfortunately, high orders are sometimes achieved at the expense of robustness: some slow algorithms are more robust than their faster counterparts.

Convergence of Newton's method

Newton's method may fail to converge. For instance



Starting from $x^{(0)}$, Newton's method diverges by taking steps that are increasingly distant from the true root, x^*. In contrast, the bisection method would converge in this case.

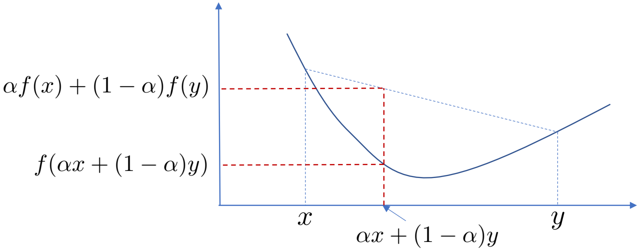
When does Newton's method converge?

First theorem

Theorem

If g' has two continuous derivatives and $g''(x^*) \neq 0$, then there exists a neighborhood of x^* for which NM converges to x^* when started from some $x^{(0)}$ in that neighborhood.

Convex function



Definition

A real-valued function f defined on an interval I is convex if the line segment between any two points on the graph of the function lies above or on the graph,

$$\forall x, y \in I, \forall \alpha \in [0,1],\ f(\alpha x+(1-\alpha)y) \leq \alpha f(x)+(1-\alpha)f(y)$$

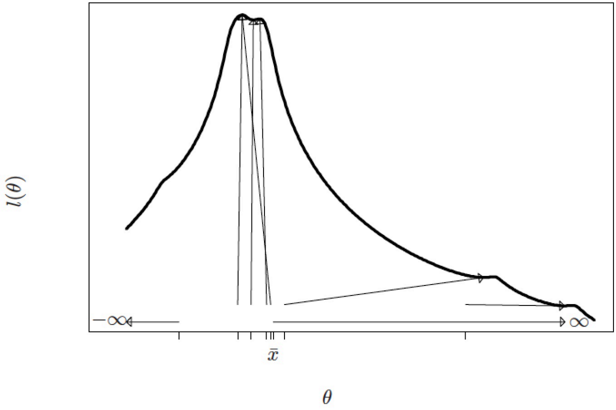
When does Newton's method converge?

Second theorem

Theorem

If g' is twice continuously differentiable, is convex and has a root, then NM converges to that root from any starting point.

Importance of the starting point



Log-likelihood for the Cauchy data. Arrows show convergence of Newton's method from several starting values

Case of maximum likelihood estimation (MLE)

- When the optimization of g corresponds to a MLE problem, where $\widehat{\theta}$ is a solution to $\ell'(\theta) = 0$, the updating equation for Newton's method is

$$\theta^{(t+1)} = \theta^{(t)} - \frac{\ell'(\theta^{(t)})}{\ell''(\theta^{(t)})}.$$

- The Fisher scoring method consists in replacing $-\ell''(\theta^{(t)})$ by its expectation for $\theta = \theta^{(t)}$, called the Fisher information evaluated at $\theta^{(t)}$.

Fisher Scoring

- Fisher information (for scalar parameter) is

$$I(\theta) = \mathbb{E}_\theta\left[\ell'(\theta)^2\right] =^* -\mathbb{E}_\theta\left[\ell''(\theta)\right]$$

  *under regularity conditions.

- Reminder: for large iid samples, it holds approximately that $\widehat{\theta} \sim \mathcal{N}\left(\theta, I(\theta)^{-1}\right)$.
- $I(\theta)$ can be approximated by $I(\widehat{\theta})$, or by $I_{obs}(\widehat{\theta}) = -\ell''(\widehat{\theta})$ (observed information). Usually $I(\widehat{\theta}) \approx I_{obs}(\widehat{\theta})$
- This suggests using the increment $h^{(t)} = \ell'(\theta^{(t)})/I(\theta^{(t)})$ where $I(\theta^{(t)})$ is the Fisher information evaluated at $\theta^{(t)}$.
- This yields

$$\theta^{(t+1)} = \theta^{(t)} + \frac{\ell'(\theta^{(t)})}{I(\theta^{(t)})}$$

Fisher Scoring vs. Newton's method

- Fisher scoring (FS) and Newton's method (NM) share the same asymptotic properties; either may be easier for a particular problem.
- In particular, $I(\theta)$ may be easier to compute. In the case of iid data, $I_n(\theta) = nI_1(\theta)$.
- The observed information $-\ell''(\theta)$ may be negative (resulting in divergence), specially far from the solution, whereas $I(\theta)$ is always positive.
- Generally, FS makes rapid improvements initially, while NM gives better refinements near the end.
- Case of the linear canonical one-parameter exponential family:

$$f(x;\theta) = b(x) \exp\left[\theta t(x) - c(\theta)\right]$$

We have $-\ell''(\theta) = c''(\theta) = I(\theta)$: FS and NM coincide.

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Secant Method

- When differentiating g' is difficult, we can replace the derivative by the discrete differenced approximation,

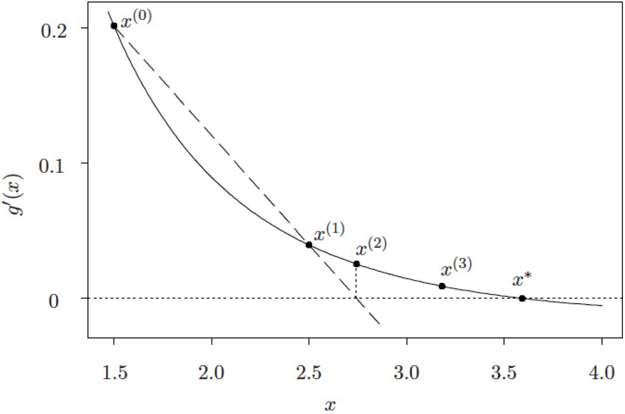
$$g''(x^{(t)}) \approx \frac{g'(x^{(t)}) - g'(x^{(t-1)})}{x^{(t)} - x^{(t-1)}}$$

- This yields the update

$$x^{(t+1)} = x^{(t)} - g'(x^{(t)}) \frac{x^{(t)} - x^{(t-1)}}{g'(x^{(t)}) - g'(x^{(t-1)})}$$

  for $t \geq 1$.
- Requires two starting points, $x^{(0)}$ and $x^{(1)}$.
- The following figure illustrates the first steps of the method for maximizing the simple function of Example 1.
- The order of convergence of the secant method is superlinear: $\beta \approx 1.62$.

Example



The secant method locally approximates g' using the secant line between $x^{(0)}$ and $x^{(1)}$. The corresponding estimated root, $x^{(2)}$, is used with $x^{(1)}$ to generate the next approximation

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Multivariate optimization for smooth g

- Let $g : \boldsymbol{x} \in \mathbb{R}^p \to \mathbb{R}$
- Stopping criteria:

$$D(\mathbf{x}^{(t+1)}, \mathbf{x}^{(t)}) < \epsilon, \quad \frac{D(\mathbf{x}^{(t+1)}, \mathbf{x}^{(t)})}{D(\mathbf{x}^{(t)}, \mathbf{0})} < \epsilon,$$

  or

$$\frac{D(\mathbf{x}^{(t+1)}, \mathbf{x}^{(t)})}{D(\mathbf{x}^{(t)}, \mathbf{0}) + \epsilon} < \epsilon.$$

  for $D(\mathbf{u}, \mathbf{v}) = \sum_{i=1}^p |u_i - v_i|$ or $D(\mathbf{u}, \mathbf{v}) = \sqrt{\sum_{i=1}^p (u_i - v_i)^2}$.

- Same strategy of iterative approximation. We will extend previous methods and introduce new options.

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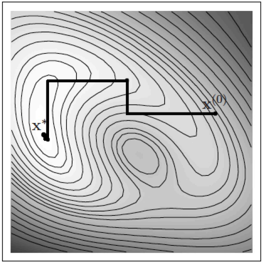
Cyclic coordinate ascent

- Also called backfitting or Gauss-Seidel iteration. One key application is for fitting additive models, GAMs, etc.
- Idea: transform a p-dimensional optimization problem into p univariate optimization problems. How?

Cyclic coordinate ascent

- Also called backfitting or Gauss-Seidel iteration. One key application is for fitting additive models, GAMs, etc.
- Idea: transform a p-dimensional optimization problem into p univariate optimization problems. How?
- Approach: optimize g with respect to each component of $\mathbf{x}$ successively, fixing all other components to their last obtained value.

Algorithm



Case $p = 2$:

- Initialize $x_1 = x_1^{(0)}$
- Find $x_2^{(1)} = \arg\max_{x_2} g(x_1^{(0)}, x_2)$
- Find $x_1^{(1)} = \arg\max_{x_1} g(x_1, x_2^{(1)})$
- Find $x_2^{(2)} = \arg\max_{x_2} g(x_1^{(1)}, x_2)$
- $\vdots$

Cyclic coordinate ascent: pros and cons

- Advantages:
  1. Simplifies a potentially difficult problem
  2. Solution of each univariate problem is easier and more stable
- Drawbacks
  1. Convergence is not guaranteed
  2. Can be slow
- For hard problems (high dimension, complex function shape), we need more sophisticated optimization procedures.

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Gradient ascent

- Gradient methods are based on the gradient

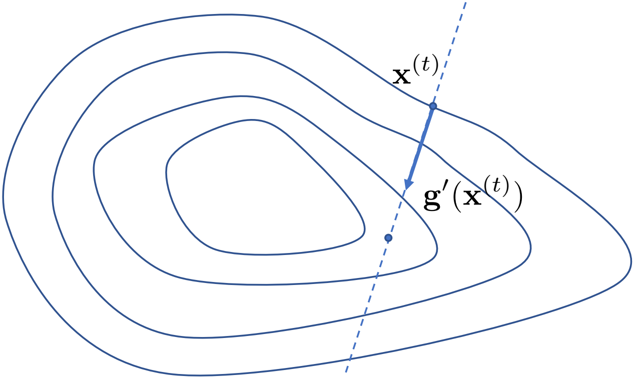
$$\mathbf{g}'(\mathbf{x}) = \left(\frac{\partial g(\mathbf{x})}{\partial x_1}, \ldots, \frac{\partial g(\mathbf{x})}{\partial x_p}\right)^T,$$

  which indicates the direction of steepest ascent of function g at $\mathbf{x}$.
- The steepest ascent method uses the update equation

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} + \alpha^{(t)} \mathbf{g}'(\mathbf{x}^{(t)}),$$

  where $\alpha^{(t)}$ is the step size at iteration t. (See next slide)
- How to determine the step size?

Gradient ascent



Ascent property

- For small enough $\alpha^{(t)}$, we have $g(\mathbf{x}^{(t+1)}) > g(\mathbf{x}^{(t)})$.
- Proof: we have

$$\begin{aligned} g(\mathbf{x}^{(t+1)}) - g(\mathbf{x}^{(t)}) &= g(\mathbf{x}^{(t)} + \alpha^{(t)}\mathbf{g}'(\mathbf{x}^{(t)})) - g(\mathbf{x}^{(t)}) \qquad (2) \\ &= \alpha^{(t)}\mathbf{g}'(\mathbf{x}^{(t)})^T\mathbf{g}'(\mathbf{x}^{(t)}) + o(\alpha^{(t)}), \qquad (3) \end{aligned}$$

where the second equality follows from the linear Taylor expansion

$$g(\mathbf{x}^{(t)} + \alpha^{(t)}\mathbf{g}'(\mathbf{x}^{(t)})) = g(\mathbf{x}^{(t)}) + \alpha^{(t)}\mathbf{g}'(\mathbf{x}^{(t)})^T\mathbf{g}'(\mathbf{x}^{(t)}) + o(\alpha^{(t)}),$$

with $o(\alpha^{(t)})/\alpha^{(t)} \to 0$ as $\alpha^{(t)} \to 0$.

- Therefore, ascent can be ensured by choosing $\alpha^{(t)}$ sufficiently small, yielding

$$g(\mathbf{x}^{(t+1)}) - g(\mathbf{x}^{(t)}) > 0$$

from (3).

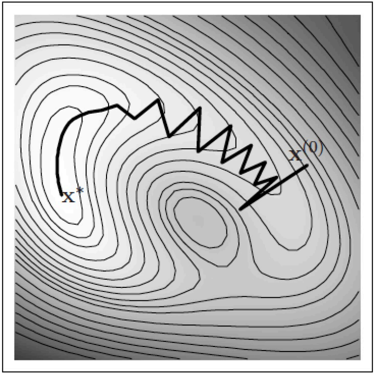
Determining $\alpha^{(t)}$

- Choosing $\alpha^{(t)}$ very small guarantees ascent, but can result in very slow convergence.
- We need a strategy to adapt $\alpha^{(t)}$, making it as large as possible, while ensuring uphill steps. Three widely used strategies:

1. Backtracking: attempt a step for, say, $\alpha^{(t)} = 1$:
    - If it is downhill, backtrack and reduce (e.g.,halve) $\alpha^{(t)}$.
    - If the step is still downhill, continue halving $\alpha^{(t)}$ until a sufficiently small step is found to be uphill.
2. Step adaptation: attempt a step with the current value $\alpha^{(t)}$;
    - If it is downhill, backtrack and set $\alpha^{(t+1)} = b\alpha^{(t)}$ with $b < 1$.
    - If it is uphill, keep the last move and set $\alpha^{(t+1)} = a\alpha^{(t)}$ with $a > 1$
3. Line search: search the $\alpha^{(t)}$ that maximizes g along the direction of the gradient:

$$\alpha^{(t)} = \arg\max_{\alpha} g(\mathbf{x}^{(t)} + \alpha \mathbf{g}'(\mathbf{x}^{(t)}))$$

Example



Steepest ascent with backtracking, using $\alpha = 0.25$ initially at each step

The steepest ascent direction is not necessarily the wisest, and backtracking doesn't prevent oversteps

Overview

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Multivariate Newton's method

- The gradient direction is not always the best.
- For instance, if g is quadratic,

$$g(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{A}\mathbf{x} + \mathbf{b}^T\mathbf{x} + c$$

with $\mathbf{A}$ negative definite, the gradient has the following expression

$$\mathbf{g}'(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$$

- Consequently, the unique maximum is found by

$$\mathbf{g}'(\mathbf{x}^*) = \mathbf{0} \Leftrightarrow \mathbf{x}^* = -\mathbf{A}^{-1}\mathbf{b}$$

Multivariate Newton's method (continued)

- This maximum can be found in one step from any starting point $\mathbf{x}^{(0)}$ by

$$\mathbf{x}^* = \mathbf{x}^{(0)} - \mathbf{g}''(\mathbf{x}^{(0)})^{-1}\mathbf{g}'(\mathbf{x}^{(0)}) \tag{4}$$

where $\mathbf{g}''(\mathbf{x}) = \left(\frac{\partial^2 g(\mathbf{x})}{\partial x_i \partial x_j}\right) = \mathbf{A}$ is the $p \times p$ Hessian matrix of g at $\mathbf{x}$.

- Indeed,

$$\mathbf{x}^{(0)} - \mathbf{g}''(\mathbf{x}^{(0)})^{-1}\mathbf{g}'(\mathbf{x}^{(0)}) = \mathbf{x}^{(0)} - \mathbf{A}^{-1}(\mathbf{A}\mathbf{x}^{(0)} + \mathbf{b}) = -\mathbf{A}^{-1}\mathbf{b}$$

- Newton's method: at each time step, approximate $g(\mathbf{x})$ around $\mathbf{x}^{(t)}$ by a second-order Taylor series expansion, and use update equation (4).

Multivariate Newton's method and Fisher scoring

- 2nd order approximation of $g(\mathbf{x})$ around $\mathbf{x}^{(t)}$:

$$g(\mathbf{x}) \approx g(\mathbf{x}^{(t)}) + (\mathbf{x} - \mathbf{x}^{(t)})^T \mathbf{g}'(\mathbf{x}^{(t)}) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(t)})^T \mathbf{g}''(\mathbf{x}^{(t)})(\mathbf{x} - \mathbf{x}^{(t)}).$$

- Setting $\mathbf{g}'(\mathbf{x}) = \mathbf{0}$, we get the update equation

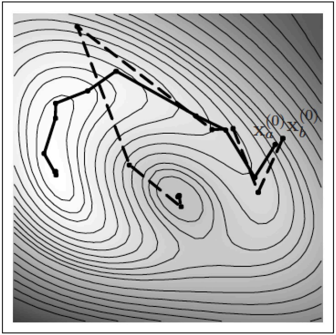
$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \mathbf{g}''(\mathbf{x}^{(t)})^{-1}\mathbf{g}'(\mathbf{x}^{(t)}).$$

- Fisher scoring:

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} + \mathbf{I}(\boldsymbol{\theta}^{(t)})^{-1}\boldsymbol{\ell}'(\boldsymbol{\theta}^{(t)}),$$

where $\mathbf{I}(\boldsymbol{\theta}) = -\mathbb{E}_{\boldsymbol{\theta}}\left[\boldsymbol{\ell}''(\boldsymbol{\theta})\right]$ is the Fisher information matrix at $\boldsymbol{\theta}$.

Example



Two runs starting from $\mathbf{x}_a^{(0)}$ and $\mathbf{x}_b^{(0)}$ are shown. These converge to the true maximum and to a local minimum, respectively.

Newton's method is not guaranteed to walk uphill. It is not guaranteed to find a local maximum. Step length matters even when step direction is good.

Newton-like methods

- Some very effective methods rely on update equations of the form

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \left(\mathbf{M}^{(t)}\right)^{-1} \mathbf{g}'(\mathbf{x}^{(t)})$$

  where $\mathbf{M}^{(t)}$ is a $p \times p$ matrix approximating the Hessian, $\mathbf{g}''(\mathbf{x}^{(t)})$.
- Two issues:
  - We want to avoid calculating the Hessian if it is computationally expensive or analytically difficult
  - We want to guarantee uphill steps

Ascent algorithms

- If we use the updating increment

$$\mathbf{h}^{(t)} = -\alpha^{(t)}\left[\mathbf{M}^{(t)}\right]^{-1}\mathbf{g}'(\mathbf{x}^{(t)}).$$

  then any positive definite matrix $-\mathbf{M}^{(t)}$ will ensure ascent for a sufficiently small $\alpha^{(t)}$
- Backtracking can be used, as in the steepest ascent method.
- Steepest ascent is recovered as a special case, with $\mathbf{M}^{(t)} = -\mathbf{I}$.
- Fisher scoring is another special case with $-\mathbf{M}^{(t)} = \mathbf{I}(\boldsymbol{\theta}^{(t)})$. Since $\mathbf{I}(\boldsymbol{\theta}^{(t)})$ is positive semi-definite, backtracking with Fisher scoring avoids stepping downhill.

Discrete Newton method

- To avoid calculating the Hessian, one could resort to an analogue of the 1-dimensional secant method.
- For example,

$$\mathbf{M}_{ij}^{(t)} = \frac{g_i'\left(\mathbf{x}^{(t)} + h_{ij}^{(t)}\mathbf{e}_j\right) - g_i'\left(\mathbf{x}^{(t)}\right)}{h_{ij}^{(t)}} \approx \frac{\partial^2 g(\mathbf{x}^{(t)})}{\partial x_i \partial x_j}$$

  where $g_i'(\mathbf{x}) = \partial g(\mathbf{x})/\partial x_i$ is the ith element of $\mathbf{g}'(\mathbf{x})$, $\mathbf{e}_j$ is the p-vector with a 1 in the jth position and zeros elsewhere, and $h_{ij}^{(t)}$ are some constants.
- $h_{ij}^{(t)} = h$ for all (i,j) and t leads to linear convergence order: $\beta = 1$.
- Alternatively, $h_{ij}^{(t)} = x_j^{(t)} - x_j^{(t-1)}$ for all i gives superlinear convergence.

Quasi-Newton methods

- The discrete Newton method strategy is computationally burdensome because $\mathbf{M}^{(t)}$ is wholly updated at every step.
- A more efficient approach can be designed based on the direction of the most recent step. From a first order Taylor series expansion of $\mathbf{g}'$ about $\mathbf{x}^{(t)}$, we have

$$\mathbf{g}'(\mathbf{x}^{(t+1)}) - \mathbf{g}'(\mathbf{x}^{(t)}) \approx \mathbf{g}''(\mathbf{x}^{(t)})(\mathbf{x}^{(t+1)} - \mathbf{x}^{(t)})$$

- $\mathbf{M}^{(t+1)}$ satisfies the secant condition if

$$\mathbf{g}'(\mathbf{x}^{(t+1)}) - \mathbf{g}'(\mathbf{x}^{(t)}) = \mathbf{M}^{(t+1)}(\mathbf{x}^{(t+1)} - \mathbf{x}^{(t)}). \tag{5}$$

- Goal: generate $\mathbf{M}^{(t+1)}$ from $\mathbf{M}^{(t)}$ in a manner that requires few calculations and satisfies (5), while learning about the curvature of $\mathbf{g}$ in the direction of the most recent step.

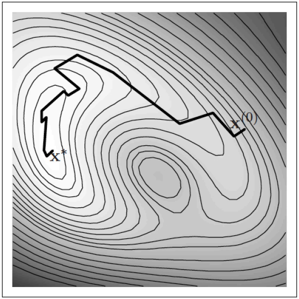
BFGS method

- The widely used BFGS method updates matrix $\mathbf{M}^{(t)}$ so as to satisfy the secant condition. It is defined by the following update equation

$$\mathbf{M}^{(t+1)} = \mathbf{M}^{(t)} - \frac{\mathbf{M}^{(t)}\mathbf{z}^{(t)}(\mathbf{M}^{(t)}\mathbf{z}^{(t)})^T}{(\mathbf{z}^{(t)})^T\mathbf{M}^{(t)}\mathbf{z}^{(t)}} + \frac{\mathbf{y}^{(t)}(\mathbf{y}^{(t)})^T}{(\mathbf{z}^{(t)})^T\mathbf{y}^{(t)}}$$

  where $\mathbf{z}^{(t)} = \mathbf{x}^{(t+1)} - \mathbf{x}^{(t)}$ and $\mathbf{y}^{(t)} = \mathbf{g}'(\mathbf{x}^{(t+1)}) - \mathbf{g}'(\mathbf{x}^{(t)})$.
- The BFGS update confers hereditary positive definiteness: if $-\mathbf{M}^{(t)}$ is positive definite, so is $-\mathbf{M}^{(t+1)}$.
- Backtracking is normally used.

Example



Quasi-Newton optimization with the BFGS update and backtracking to ensure ascent.

Convergence of quasi-Newton methods is generally superlinear, but not quadratic. These are powerful and popular methods, available, for example, in the R function `optim()`.

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Basic idea

- Consider a nonlinear least squares problem with observed data $(\mathbf{z}_i, y_i)$ for $i = 1, \ldots, n$ and model

$$Y_i = f(\mathbf{z}_i, \boldsymbol{\theta}) + \epsilon_i$$

  for some non-linear function, f, and random error, ϵ_i.
- We seek to estimate $\boldsymbol{\theta}$ by maximizing an objective function

$$g(\boldsymbol{\theta}) = -\sum_{i=1}^{n} (y_i - f(\mathbf{z}_i, \boldsymbol{\theta}))^2 .$$

- Newton's method approximates g via Taylor series. The Gauss-Newton approach approximates f itself by its linear Taylor series expansion about $\boldsymbol{\theta}^{(t)}$.

Linearized reformulation

- We have

$$f(\mathbf{z}_i, \boldsymbol{\theta}) \approx f(\mathbf{z}_i, \boldsymbol{\theta}^{(t)}) + (\boldsymbol{\theta} - \boldsymbol{\theta}^{(t)})^T \mathbf{f}'(\mathbf{z}_i, \boldsymbol{\theta}^{(t)})$$

  where for each i, $\mathbf{f}'(\mathbf{z}_i, \boldsymbol{\theta}^{(t)})$ is the column vector of partial derivatives of f with respect to θ_j, for $j = 1, \ldots, p$, evaluated at $(\mathbf{z}_i, \boldsymbol{\theta}^{(t)})$.

- Now, instead of $g(\boldsymbol{\theta})$, we maximize

$$\begin{aligned}\tilde{g}(\boldsymbol{\theta}) &= -\sum_{i=1}^{n} \left(\underbrace{y_i - f(\mathbf{z}_i, \boldsymbol{\theta}^{(t)})}_{x_i^{(t)}} - (\boldsymbol{\theta} - \boldsymbol{\theta}^{(t)})^T \underbrace{\mathbf{f}'(\mathbf{z}_i, \boldsymbol{\theta}^{(t)})}_{\mathbf{a}_i^{(t)}} \right)^2 \\ &= -\sum_{i=1}^{n} \left(x_i^{(t)} - (\boldsymbol{\theta} - \boldsymbol{\theta}^{(t)})^T \mathbf{a}_i^{(t)} \right)^2\end{aligned}$$

  with respect to $\boldsymbol{\theta}$.

Update equation

- Then the approximated problem can be re-expressed as minimizing the squared residuals of the linear regression model

$$\underbrace{\mathbf{x}^{(t)}}_{\text{response}} = \underbrace{\mathbf{A}^{(t)}}_{\text{design matrix}} \underbrace{(\boldsymbol{\theta} - \boldsymbol{\theta}^{(t)})}_{\text{coefficients}} + \boldsymbol{\epsilon}$$

where $\mathbf{x}^{(t)}$ and $\boldsymbol{\epsilon}$ are column vectors whose ith elements consist of $x_i^{(t)}$ and ϵ_i, respectively. Similarly, $\mathbf{A}^{(t)}$ is a matrix whose ith row is $(\mathbf{a}_i^{(t)})^T$.

- The solution is

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} + \left((\mathbf{A}^{(t)})^T \mathbf{A}^{(t)}\right)^{-1} (\mathbf{A}^{(t)})^T \mathbf{x}^{(t)}.$$

- The method requires no computation of Hessian.
- It works best when the model fits fairly well and f is not severely nonlinear.

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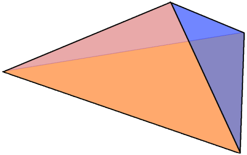
Main idea

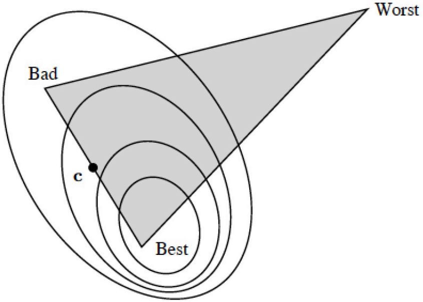
- An algorithm that does not require the calculation of $\mathbf{g}'(\mathbf{x})$ or $\mathbf{g}''(\mathbf{x})$.
- Idea: evaluate g at $p+1$ points $\mathbf{x}_1, \ldots, \mathbf{x}_{p+1}$ forming a simplex*.
- This simplex defines a region, which is iteratively reshaped by replacing the worst point (vertex) by a better one.

Definition (*k-simplex)

A k-simplex is a k-dimensional polytope which is the convex hull of $k+1$ points (vertices). A a 2-simplex is a triangle. A 3-simplex is a tetrahedron.



Definitions

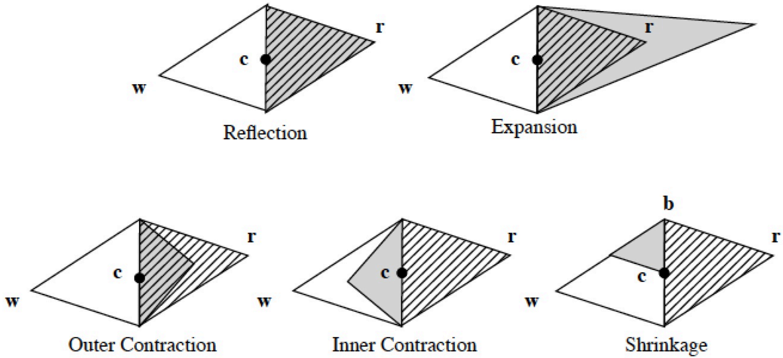


Let

- $\mathbf{x}_{best}$: vertex with highest value of g
- $\mathbf{x}_{worst}$: vertex with lowest value of g
- $\mathbf{x}_{bad}$: 2nd worst vertex
- Best face: face opposite to $\mathbf{x}_{worst}$, $\mathbf{c}$ its centroid.

Transformations of a vertex

Five possible transformations of a vertex by replacing $\mathbf{x}_{worst}$:



Reflection

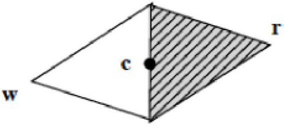
Expansion

Outer Contraction

Inner Contraction

Shrinkage

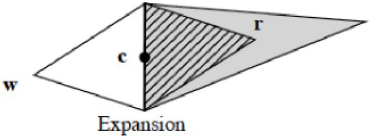
Basic algorithm



Reflection

- The location of the new vertex (replacing $\mathbf{x}_{worst}$) is based on the reflection vertex $\mathbf{x}_r = \mathbf{c} + \alpha_r(\mathbf{c} - \mathbf{x}_{worst})$, usually $\alpha_r = 1$
- If $g(\mathbf{x}_{bad}) < g(\mathbf{x}_r) < g(\mathbf{x}_{best})$: keep $\mathbf{x}_r$ as the new vertex
- If $g(\mathbf{x}_r) > g(\mathbf{x}_{best})$: try an expansion step
- If $g(\mathbf{x}_r) < g(\mathbf{x}_{bad})$: try a contraction step

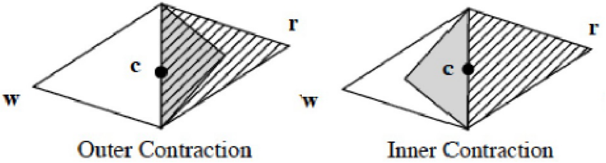
Expansion



If $g(\mathbf{x}_r) > g(\mathbf{x}_{best})$: Expansion.
Let $\mathbf{x}_e = \mathbf{c} + \alpha_e(\mathbf{x}_r - \mathbf{c})$, usually $\alpha_e = 2$

- If $g(\mathbf{x}_e) > g(\mathbf{x}_r)$: set $\mathbf{x}_e$ as the new vertex
- Otherwise, keep $\mathbf{x}_r$

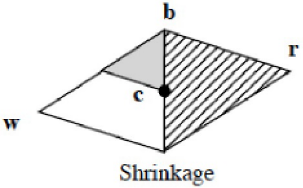
Contraction



If $g(\mathbf{x}_r) < g(\mathbf{x}_{bad})$: Contraction.

- If $g(\mathbf{x}_r) > g(\mathbf{x}_{worst})$: outer contraction. Let $\mathbf{x}_o = \mathbf{c} + \alpha_c(\mathbf{x}_r - \mathbf{c})$, usually $\alpha_c = 0.5$.
  - If $g(\mathbf{x}_o) > g(\mathbf{x}_r)$: keep $\mathbf{x}_o$
  - Otherwise: perform a shrink transformation
- If $g(\mathbf{x}_r) \leq g(\mathbf{x}_{worst})$: inner contraction. Let $\mathbf{x}_i = \mathbf{c} + \alpha_c(\mathbf{x}_{worst} - \mathbf{c})$.
  - If $g(\mathbf{x}_i) > g(\mathbf{x}_{worst})$: keep $\mathbf{x}_i$
  - Otherwise: perform a shrink transformation

Shrinking

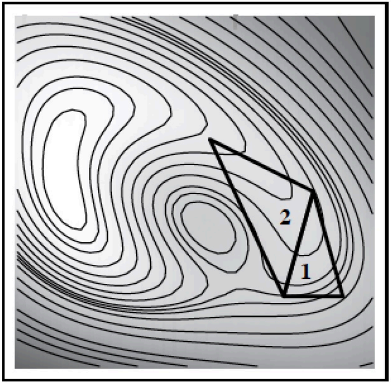


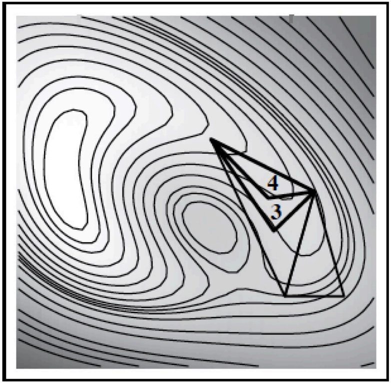
Shrink transformation: all vertices except x_{best} are shrunk toward x_{best}:

$$\mathsf{x}'_j = \mathsf{x}_{best} + \alpha_s(\mathsf{x}_j - \mathsf{x}_{best}),$$

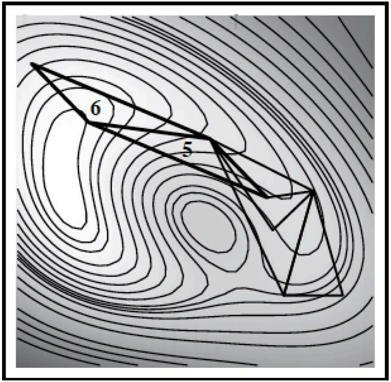
usually $\alpha_s = 0.5$.

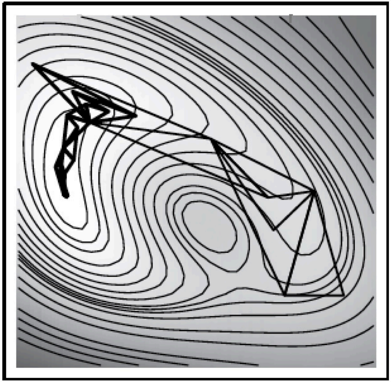
Example





Example (continued)





Performance of the Nelder-Mead algorithm

- The NM method is generally quite good at finding optima, especially for low to moderate dimensions. For high-dimensional problems, its effectiveness is more varied, depending on the nature of the problem.
- The NM approach is quite robust in the sense that it can successfully find optima for a wide range of functions – even discontinuous ones – and from a wide range of starting values. Moreover, it is robust in the sense that convergence is often not much impeded when the objective function values are contaminated with random noise.
- Despite its good performance, the NM algorithm can perform poorly in certain circumstances. It is even possible for the algorithm to converge to points that are neither local maxima nor minima.